Tensor Properties of Materials

Bálint Koczor

– 2023 –

UNIVERSITY OF OXFORD

NOTICE OF LECTURE RECORDING

- This session is being recorded and will be available for students to view on-demand. The recording will be stored in the Panopto cloud and will be accessible using your SSO via Canvas/WebLearn (delete as appropriate). Access to this recording is restricted to students in this year group and registered on this course.

- Please be aware that all screen activity, including any active webcams/mics that are visible and/or audible, may be recorded.

For more information about lecture recording at the University, please consult the University's Lecture Recording Policy.

If you have any questions or concerns, please email **replay@it.ox.ac.uk**

1. Basic principles
   - Properties and variables
   - Scalar and vector variables
   - Tensor properties
   - Crystal symmetry, Neumann's principle
   - Transformation of coordinates, transformation of vectors and tensors
   - Representation surface, principal axes
2. Second-rank tensors
   - Thermal and electrical conductivity
   - Electrical and magnetic susceptibility
   - Stress and strain
   - Thermal expansion
   - Optical properties of crystals
3. Third and fourth-rank tensors
   - Piezoelectricity
   - Elastic stiffness and compliance
   - Elastic properties of cubic and isotropic crystals

Linear response in materials

effect		proportionality (property of material)	cause (external)
current density J	$=$	conductivity σ	electric field E
el. polaris. P	$=$	el. suscept. $\epsilon_0 \chi$	electric field E
thermal exp. ϵ	$=$	thermal exp. coeff. α	change of temp. ΔT
stress σ	$=$	stiffness C	strain ϵ

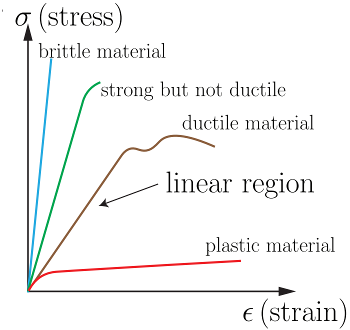
Linear response in materials

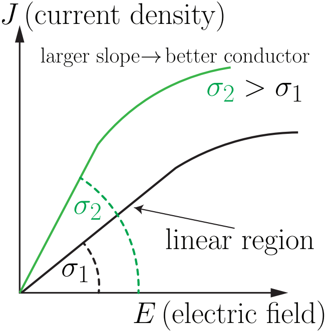
effect		proportionality (property of material)	cause (external)
current density J	$=$	conductivity σ	electric field E
el. polaris. P	$=$	el. suscept. $\epsilon_0\chi$	electric field E
thermal exp. ϵ	$=$	thermal exp. coeff. α	change of temp. ΔT
stress σ	$=$	stiffness C	strain ϵ

- valid only in 1D – we need to go beyond numbers J, P etc.
- a physical quantity has both magnitude and direction
- linear relations in vector fields $\vec{J} = \sigma\vec{E}$

Linear approximation

deviation from linear: too large current → thermal effects, breakdown

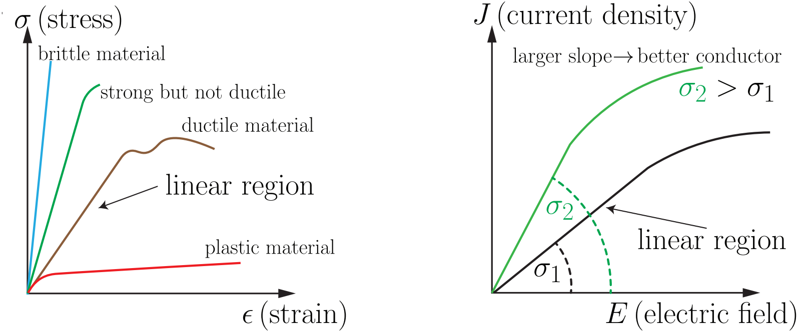




- when cause is 'small' then effect is linear via a Taylor series $f(x) = f(0) + f'(0)x + \dots$
- slope $f'(x) = \sigma$ is the proportionality: property of the material

Linear approximation

deviation from linear: too large current → thermal effects, breakdown



- when cause is 'small' then effect is linear via a Taylor series $f(x) = f(0) + f'(0)x + \ldots$
- slope $f'(x) = \sigma$ is the proportionality: property of the material
- in isotropic material σ independent of direction of $\vec{E}$
- **linear** but anistropic material: we need to use tensors

isotropic material

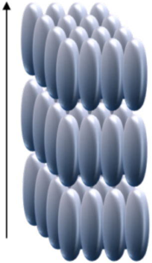
- macroscopic properties **independent of direction**
- amorphous materials: glass
- small-grained polycrystalline materials: averaging
- some crystals: linear response in cubic crystals
- proportional vectors $\vec{J} = \sigma \vec{E}$

isotropic material

- macroscopic properties **independent of direction**
- amorphous materials: glass
- small-grained polycrystalline materials: averaging
- some crystals: linear response in cubic crystals
- proportional vectors $\vec{J} = \sigma \vec{E}$

anisotropic material

- macroscopic properties **depend on direction**
- liquid crystals
- fibre composites: wood, reinforced concrete
- single crystals: most crystal lattices
- need to write $\vec{J} = \text{tensor} \cdot \vec{E}$



Applications of anisotropy

anisotropy is the key to so many technologies and applications

Piezoelectricity

- quartz oscillators – clock frequency in computers
- gas lighters
- stepper motors and high-precision positioning
- sensors – microphones

Optical devices

- polarisers
- beam splitters

Liquid crystals

- LCD screen, displays
- watch
- etc.

Thought experiment in anisotropic materials

vector $\vec{J} = (J_x, J_y, J_z)$ not necessarily **parallel** to $\vec{E} = (E_x, E_y, E_z)$

- we apply electric field $\vec{E}$ to anisotropic material (**cause**)
- measure the resulting current density vector $\vec{J}$ (**effect**)
- linearity: $2\vec{E}$ results in $2\vec{J}$ with same direction

Thought experiment in anisotropic materials

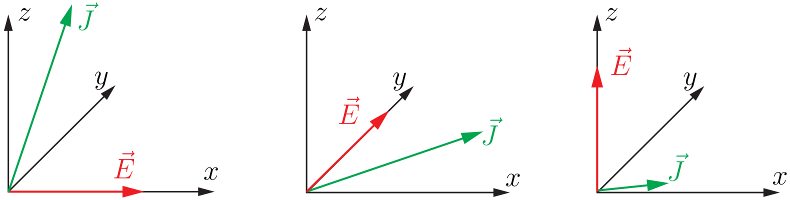
vector $\vec{J} = (J_x, J_y, J_z)$ not necessarily **parallel** to $\vec{E} = (E_x, E_y, E_z)$

- we apply electric field $\vec{E}$ to anisotropic material (**cause**)
- measure the resulting current density vector $\vec{J}$ (**effect**)
- linearity: $2\vec{E}$ results in $2\vec{J}$ with same direction

x direction

apply $\vec{E} = E_x \vec{x}$

$$J_x = \sigma_{xx} E_x$$
$$J_y = \sigma_{yx} E_x$$
$$J_z = \sigma_{zx} E_x$$

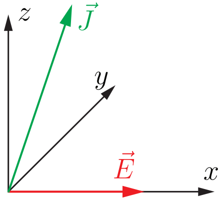


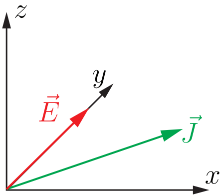
Thought experiment in anisotropic materials

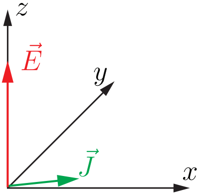
vector $\vec{J} = (J_x, J_y, J_z)$ not necessarily **parallel** to $\vec{E} = (E_x, E_y, E_z)$

- we apply electric field $\vec{E}$ to anisotropic material (**cause**)
- measure the resulting current density vector $\vec{J}$ (**effect**)
- linearity: $2\vec{E}$ results in $2\vec{J}$ with same direction

x direction	y direction
apply $\vec{E} = E_x\vec{x}$	apply $\vec{E} = E_y\vec{y}$
$J_x = \sigma_{xx} E_x$	$J_x = \sigma_{xy} E_y$
$J_y = \sigma_{yx} E_x$	$J_y = \sigma_{yy} E_y$
$J_z = \sigma_{zx} E_x$	$J_z = \sigma_{zy} E_y$







Thought experiment in anisotropic materials

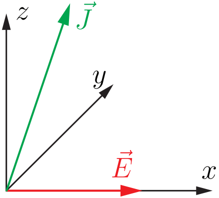
vector $\vec{J} = (J_x, J_y, J_z)$ not necessarily **parallel** to $\vec{E} = (E_x, E_y, E_z)$

- we apply electric field $\vec{E}$ to anisotropic material (**cause**)
- measure the resulting current density vector $\vec{J}$ (**effect**)
- linearity: $2\vec{E}$ results in $2\vec{J}$ with same direction

x direction

apply $\vec{E} = E_x\vec{x}$

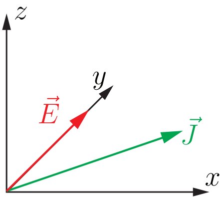
$$J_x = \sigma_{xx}E_x$$
$$J_y = \sigma_{yx}E_x$$
$$J_z = \sigma_{zx}E_x$$



y direction

apply $\vec{E} = E_y\vec{y}$

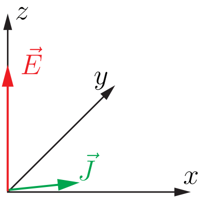
$$J_x = \sigma_{xy}E_y$$
$$J_y = \sigma_{yy}E_y$$
$$J_z = \sigma_{zy}E_y$$



z direction

apply $\vec{E} = E_z\vec{z}$

$$J_x = \sigma_{xz}E_z$$
$$J_y = \sigma_{yz}E_z$$
$$J_z = \sigma_{zz}E_z$$



Writing linear equations compactly

linearity: if we apply $\vec{E} = (E_x, E_y, E_z)$ we sum x, y, z contributions

$$J_x = \sigma_{xx} E_x + \sigma_{xy} E_y + \sigma_{xz} E_z,$$
$$J_y = \sigma_{yx} E_x + \sigma_{yy} E_y + \sigma_{yz} E_z$$
$$J_z = \sigma_{zx} E_x + \sigma_{zy} E_y + \sigma_{zz} E_z$$

Writing linear equations compactly

linearity: if we apply $\vec{E} = (E_x, E_y, E_z)$ we sum x, y, z contributions

$$J_x = \sigma_{xx}E_x + \sigma_{xy}E_y + \sigma_{xz}E_z,$$
$$J_y = \sigma_{yx}E_x + \sigma_{yy}E_y + \sigma_{yz}E_z$$
$$J_z = \sigma_{zx}E_x + \sigma_{zy}E_y + \sigma_{zz}E_z$$

- notation for axes $\vec{x} = \vec{x}_1$, $\vec{y} = \vec{x}_2$ and $\vec{z} = \vec{x}_3$
- and for vector components $J_x = J_1$, $J_y = J_2$ and $J_z = J_3$
- and we denote the idexes: $i, j, k, l \cdots \in \{1, 2, 3\}$

Writing linear equations compactly

linearity: if we apply $\vec{E} = (E_x, E_y, E_z)$ we sum x, y, z contributions

$$J_x = \sigma_{xx}E_x + \sigma_{xy}E_y + \sigma_{xz}E_z,$$
$$J_y = \sigma_{yx}E_x + \sigma_{yy}E_y + \sigma_{yz}E_z$$
$$J_z = \sigma_{zx}E_x + \sigma_{zy}E_y + \sigma_{zz}E_z$$

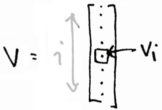
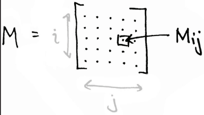
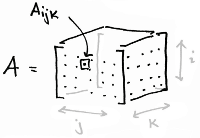
- notation for axes $\vec{x} = \vec{x}_1$, $\vec{y} = \vec{x}_2$ and $\vec{z} = \vec{x}_3$
- and for vector components $J_x = J_1$, $J_y = J_2$ and $J_z = J_3$
- and we denote the idexes: $i, j, k, l \cdots \in \{1, 2, 3\}$
- use compact **Einstein convention** or **matrix/vector prod.**

$$J_i = \sum_{j=1}^{3} \sigma_{ij}E_j \equiv \sigma_{ij}E_j$$

$$\begin{bmatrix} J_1 \\ J_2 \\ J_3 \end{bmatrix} = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} \begin{bmatrix} E_1 \\ E_2 \\ E_3 \end{bmatrix}$$

What is a tensor?

rank-r array of numbers

$r = 0$ scalar: T	$r = 1$ vector: V_i	$r = 2$ matrix: M_{ij}	$r = 3$ (3D) array: A_{ijk}
			

- very useful in so many applications
- materials: express linear properties of materials
- machine learning: tensors are weights in neural networks

TensorFlow

Matrix and vector notation

- for rank $r = 1, 2$ can use compact **matrix/vector notations**
- for rank $r \geq 2$ need to use tensors and **Einstein summation**
- Einstein convention: we imply summing over repeated indexes

explicit	Einstein conv.	matrix notation	type
$a = \sum_{i=1}^{3} v_i w_i$	$a = v_i w_i$	$a = \vec{v} \cdot \vec{w}$	vector/vector
$a_i = \sum_{j=1}^{3} T_{ij} v_j$	$a_i = T_{ij} v_j$	$\vec{a} = \mathbf{T} \cdot \vec{v}$	matrix/vector
$R_{ik} = \sum_{j=1}^{3} S_{ij} T_{jk}$	$R_{ik} = S_{ij} T_{jk}$	$\mathbf{R} = \mathbf{S} \cdot \mathbf{T}$	matrix/matrix
$R_{ij} = \sum_{k,l=1}^{3} S_{ijkl} T_{kl}$	$R_{ij} = S_{ijkl} T_{kl}$		

Matrix and vector notation

- for rank $r = 1, 2$ can use compact **matrix/vector notations**
- for rank $r \geq 2$ need to use tensors and **Einstein summation**
- Einstein convention: we imply summing over repeated indexes

explicit	Einstein conv.	matrix notation	type
$a = \sum_{i=1}^{3} v_i w_i$	$a = v_i w_i$	$a = \vec{v} \cdot \vec{w}$	vector/vector
$a_i = \sum_{j=1}^{3} T_{ij} v_j$	$a_i = T_{ij} v_j$	$\vec{a} = \mathbf{T} \cdot \vec{v}$	matrix/vector
$R_{ik} = \sum_{j=1}^{3} S_{ij} T_{jk}$	$R_{ik} = S_{ij} T_{jk}$	$\mathbf{R} = \mathbf{S} \cdot \mathbf{T}$	matrix/matrix
$R_{ij} = \sum_{k,l=1}^{3} S_{ijkl} T_{kl}$	$R_{ij} = S_{ijkl} T_{kl}$		

- tensors (as well as matrices/vectors) express linear relations
- apply electric field twice as large $\vec{E} \to 2\vec{E}$ then effect $\vec{J} \to 2\vec{J}$
- **linearity:** if we make $\sigma_{ij} \to 2\sigma_{ij}$ twice as large, same effect

Summary of lecture 1

Basic principles

- cause-effect: linear relations used when cause is small
- anisotropy: macroscopic properties depend on direction
- cause vector is not necessarily parallel to effect vector
- in this case we used tensors to express linear relations

Tensors basics

- tensors, such as T_{ijk}, are rank-r arrays of numbers
- with materials we work in 3D and indexes run for $i, j, k = 1, 2, 3$
- rank 1 and rank 2: we can use matrices and vectors
- for higher ranks we use Einstein convention: summation over repeated index is implied

NOTICE OF LECTURE RECORDING

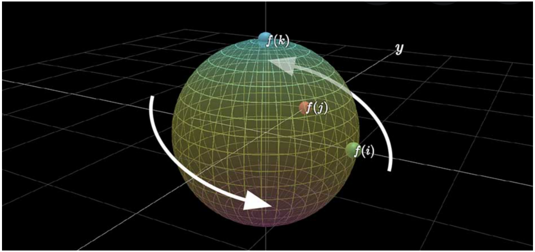
- This session is being recorded and will be available for students to view on-demand. The recording will be stored in the Panopto cloud and will be accessible using your SSO via Canvas/WebLearn (delete as appropriate). Access to this recording is restricted to students in this year group and registered on this course.
- Please be aware that all screen activity, including any active webcams/mics that are visible and/or audible, may be recorded.

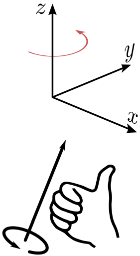
For more information about lecture recording at the University, please consult the University's Lecture Recording Policy.

If you have any questions or concerns, please email **replay@it.ox.ac.uk**

Coordinate system rotations

- isotropic materials: rotation does not affect properties
- anisotropic materials: problems simplify when viewed in specific coordinate systems – we want to apply rotations



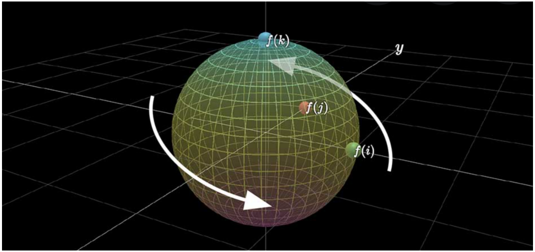


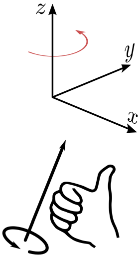
Coordinate system rotations

- isotropic materials: rotation does not affect properties
- anisotropic materials: problems simplify when viewed in specific coordinate systems – we want to apply rotations
- compactly describe rotations using rotation matrices

$$\vec{J}' = \mathbf{L}\vec{J} \qquad\qquad J_i' = L_{ij} J_j$$

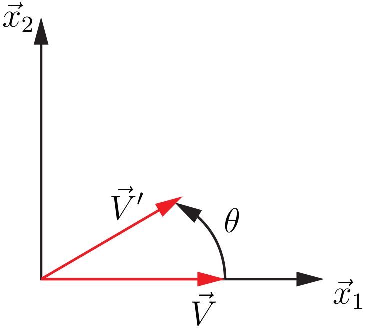
- computer graphics: rotate vectors whenever we move camera





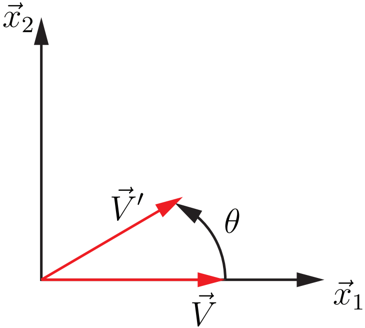
Example: matrix of rotation around z axis

Rotate vectors that are parallel with coord. axes: $V_1\vec{x_1}$, $V_2\vec{x_2}$, $V_3\vec{x_3}$



Example: matrix of rotation around z axis

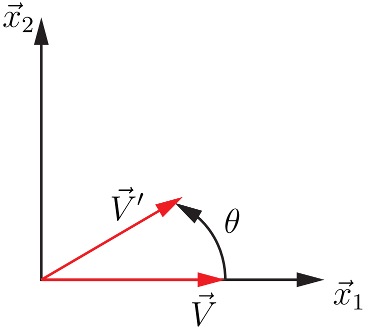
Rotate vectors that are parallel with coord. axes: $V_1\vec{x_1}$, $V_2\vec{x_2}$, $V_3\vec{x_3}$



$$\mathbf{L}\begin{bmatrix}V_1\\0\\0\end{bmatrix} = V_1\begin{bmatrix}\cos\theta\\ \sin\theta\\ 0\end{bmatrix}$$

Example: matrix of rotation around z axis

Rotate vectors that are parallel with coord. axes: $V_1\vec{x_1}$, $V_2\vec{x_2}$, $V_3\vec{x_3}$

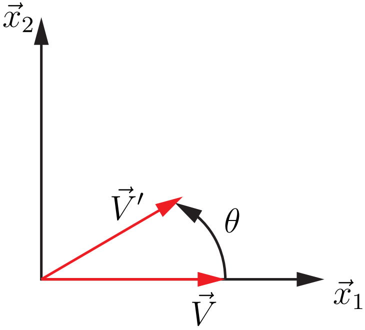


$$\mathbf{L}\begin{bmatrix}V_1\\0\\0\end{bmatrix} = V_1\begin{bmatrix}\cos\theta\\\sin\theta\\0\end{bmatrix}$$

$$\mathbf{L}\begin{bmatrix}0\\V_2\\0\end{bmatrix} = V_2\begin{bmatrix}-\sin\theta\\\cos\theta\\0\end{bmatrix}$$

Example: matrix of rotation around z axis

Rotate vectors that are parallel with coord. axes: $V_1\vec{x_1}$, $V_2\vec{x_2}$, $V_3\vec{x_3}$



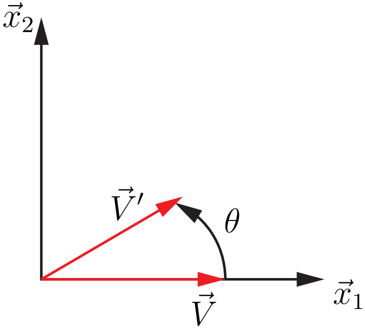
$$\mathbf{L}\begin{bmatrix}V_1\\0\\0\end{bmatrix} = V_1\begin{bmatrix}\cos\theta\\\sin\theta\\0\end{bmatrix}$$

$$\mathbf{L}\begin{bmatrix}0\\V_2\\0\end{bmatrix} = V_2\begin{bmatrix}-\sin\theta\\\cos\theta\\0\end{bmatrix}$$

$$\mathbf{L}\begin{bmatrix}0\\0\\V_3\end{bmatrix} = V_3\begin{bmatrix}0\\0\\1\end{bmatrix}$$

Example: matrix of rotation around z axis

Rotate vectors that are parallel with coord. axes: $V_1\vec{x_1}$, $V_2\vec{x_2}$, $V_3\vec{x_3}$



$$\mathbf{L}\begin{bmatrix} V_1 \\ 0 \\ 0 \end{bmatrix} = V_1 \begin{bmatrix} \cos\theta \\ \sin\theta \\ 0 \end{bmatrix}$$

$$\mathbf{L}\begin{bmatrix} 0 \\ V_2 \\ 0 \end{bmatrix} = V_2 \begin{bmatrix} -\sin\theta \\ \cos\theta \\ 0 \end{bmatrix}$$

$$\mathbf{L}\begin{bmatrix} 0 \\ 0 \\ V_3 \end{bmatrix} = V_3 \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

- a general vector is just the sum $\vec{V} = V_1\vec{x_1} + V_2\vec{x_2} + V_3\vec{x_3}$
- right-hand sides above must be column vectors of $\mathbf{L}$

$$\begin{bmatrix} V_1' \\ V_2' \\ V_3' \end{bmatrix} = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} V_1 \\ V_2 \\ V_2 \end{bmatrix}$$

Basic and general rotations

Basic rotation matrices:

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \; R_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix}, \; R_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Basic and general rotations

Basic rotation matrices:

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix},\ R_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix},\ R_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

But how about an off-axis rotation? General rot. matrix $\mathbf{L}$

$$\mathbf{L} = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix}, \qquad \mathbf{L} \text{ must be orthogonal and } \det \mathbf{L} = 1$$

Basic and general rotations

Basic rotation matrices:

$$R_x = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix},\; R_y = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix},\; R_z = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

But how about an off-axis rotation? General rot. matrix $\mathbf{L}$

$$\mathbf{L} = \begin{bmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{bmatrix}, \qquad \mathbf{L} \text{ must be orthogonal and } \det \mathbf{L} = 1$$

We can use $\mathbf{L}$ to rotate all axes $\vec{x}'_i = \mathbf{L}\vec{x}_i$ (see colour in prev. slide)

$$\vec{x}'_1 = \begin{bmatrix} L_{11} \\ L_{21} \\ L_{31} \end{bmatrix}, \qquad \vec{x}'_2 = \begin{bmatrix} L_{12} \\ L_{22} \\ L_{32} \end{bmatrix}, \qquad \vec{x}'_3 = \begin{bmatrix} L_{13} \\ L_{23} \\ L_{33} \end{bmatrix}$$

- $L_{ij} = \cos\theta_{ij}$ are scalar products between orig. and new axes
- **example:** θ_{12} is angle between original $\vec{x}_1$ and new $\vec{x}'_2$

Orthogonal matrices

- **But** new coordinate axes $\vec{x}'_i$ must be orthogonal and normalised
- **example:** $L_{i1}L_{i1} = \vec{x}'_1 \cdot \vec{x}'_1 = 1$ while $L_{i1}L_{i2} = \vec{x}'_1 \cdot \vec{x}'_2 = 0$

Orthogonal matrices

- **But** new coordinate axes $\vec{x}'_i$ must be orthogonal and normalised
- **example:** $L_{i1}L_{i1} = \vec{x}'_1 \cdot \vec{x}'_1 = 1$ while $L_{i1}L_{i2} = \vec{x}'_1 \cdot \vec{x}'_2 = 0$
- in $\mathbf{L}$ column and row vectors are mutually orthogonal

$$\boxed{\mathbf{L}^T\mathbf{L} = \mathbb{1} \qquad\qquad L_{ij}L_{ik} = \delta_{jk}}$$

- Kronecker delta $\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ otherwise
- guarantees transpose is inverse operation $\mathbf{L}^T J' = J$

Orthogonal matrices

- **But** new coordinate axes $\vec{x}'_i$ must be orthogonal and normalised
- **example:** $L_{i1}L_{i1} = \vec{x}'_1 \cdot \vec{x}'_1 = 1$ while $L_{i1}L_{i2} = \vec{x}'_1 \cdot \vec{x}'_2 = 0$
- in $\mathbf{L}$ column and row vectors are mutually orthogonal

$$\boxed{\mathbf{L}^T\mathbf{L} = \mathbb{1} \qquad\qquad L_{ij}L_{ik} = \delta_{jk}}$$

- Kronecker delta $\delta_{ij} = 1$ when $i = j$ and $\delta_{ij} = 0$ otherwise
- guarantees transpose is inverse operation $\mathbf{L}^T J' = J$

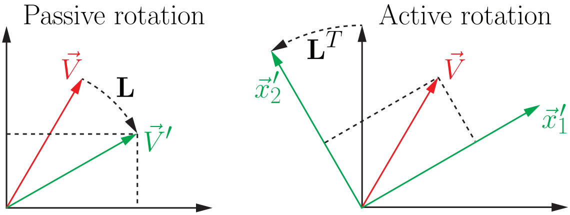
reminder: diagonalising matrices via eigenvectors

$$\mathbf{M} = \mathbf{L} \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \mathbf{L}^T$$

- diagonalise real, symmetric matrix $\mathbf{M}$ with real eigenvalues λ_i
- here $\mathbf{L}$ contains eigenvectors of $\mathbf{M}$ as columns – orthogonal

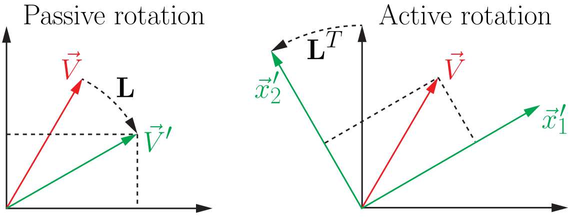
Active and Passive rotations

- so far, actively rotated vector to a new one $\vec{J}' = \mathbf{L}\vec{J}$
- physical variable $\vec{J}$ should not change, just frame of ref
- passive: vector $\vec{J}$ remains unchanged, entries wrt new coord syst



Active and Passive rotations

- so far, actively rotated vector to a new one $\vec{J}' = \mathbf{L}\vec{J}$
- physical variable $\vec{J}$ should not change, just frame of ref
- passive: vector $\vec{J}$ remains unchanged, entries wrt new coord syst



active rotation $\vec{V}' = \mathbf{L}\vec{V}$ equivalent to: passive rotation with inversely rotated coord syst $\vec{x}_i' = \mathbf{L}^T\vec{x}_i$

$$\underbrace{\begin{bmatrix} \vec{V}' \cdot \vec{x}_1 \\ \vec{V}' \cdot \vec{x}_2 \\ \vec{V}' \cdot \vec{x}_3 \end{bmatrix}}_{\text{active rotation}} = \begin{bmatrix} V_1' \\ V_2' \\ V_2' \end{bmatrix} = \underbrace{\begin{bmatrix} \vec{V} \cdot \vec{x}_1' \\ \vec{V} \cdot \vec{x}_2' \\ \vec{V} \cdot \vec{x}_3' \end{bmatrix}}_{\text{passive rotation}}$$

Rotating tensors

one coordinate system $\vec{E}$ and $\vec{J}$, in other one $\vec{E}' = \mathbf{L}\vec{E}$ and $\vec{J}' = \mathbf{L}\vec{J}$

Rotating tensors

one coordinate system $\vec{E}$ and $\vec{J}$, in other one $\vec{E}' = \mathbf{L}\vec{E}$ and $\vec{J}' = \mathbf{L}\vec{J}$

$$\vec{J} = \boldsymbol{\sigma}\vec{E} \qquad \text{substitute } \vec{J} = \mathbf{L}^T\vec{J}' \text{ and } \vec{E} = \mathbf{L}^T\vec{E}'$$

$$\mathbf{L}^T\vec{J}' = \boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{multiply with } \mathbf{L} \text{ from left}$$

$$\mathbf{L}\mathbf{L}^T\vec{J}' = \mathbf{L}\boldsymbol{\sigma}'\mathbf{L}^T\vec{E}' \qquad \text{simplify } \mathbf{L}\mathbf{L}^T = \mathbb{1}$$

$$\vec{J}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{denote } \boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$$

$$\vec{J}' = \boldsymbol{\sigma}'\vec{E}'$$

Rotating tensors

one coordinate system $\vec{E}$ and $\vec{J}$, in other one $\vec{E}' = \mathbf{L}\vec{E}$ and $\vec{J}' = \mathbf{L}\vec{J}$

$$\vec{J} = \boldsymbol{\sigma}\vec{E} \qquad \text{substitute } \vec{J} = \mathbf{L}^T\vec{J}' \text{ and } \vec{E} = \mathbf{L}^T\vec{E}'$$

$$\mathbf{L}^T\vec{J}' = \boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{multiply with } \mathbf{L} \text{ from left}$$

$$\mathbf{L}\mathbf{L}^T\vec{J}' = \mathbf{L}\boldsymbol{\sigma}'\mathbf{L}^T\vec{E}' \qquad \text{simplify } \mathbf{L}\mathbf{L}^T = \mathbb{1}$$

$$\vec{J}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{denote } \boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$$

$$\vec{J}' = \boldsymbol{\sigma}'\vec{E}'$$

Tensor entries transform due to rotation

$$\boxed{\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T \qquad \sigma'_{ij} = L_{ik}\sigma_{kl}L_{jl}}$$

Rotating tensors

one coordinate system $\vec{E}$ and $\vec{J}$, in other one $\vec{E}' = \mathbf{L}\vec{E}$ and $\vec{J}' = \mathbf{L}\vec{J}$

$$\vec{J} = \boldsymbol{\sigma}\vec{E} \qquad \text{substitute } \vec{J} = \mathbf{L}^T\vec{J}' \text{ and } \vec{E} = \mathbf{L}^T\vec{E}'$$

$$\mathbf{L}^T\vec{J}' = \boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{multiply with } \mathbf{L} \text{ from left}$$

$$\mathbf{L}\mathbf{L}^T\vec{J}' = \mathbf{L}\boldsymbol{\sigma}'\mathbf{L}^T\vec{E}' \qquad \text{simplify } \mathbf{L}\mathbf{L}^T = \mathbb{1}$$

$$\vec{J}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T\vec{E}' \qquad \text{denote } \boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$$

$$\vec{J}' = \boldsymbol{\sigma}'\vec{E}'$$

Tensor entries transform due to rotation

$$\boxed{\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T \qquad \sigma'_{ij} = L_{ik}\sigma_{kl}L_{jl}}$$

remark: formal definition of a rank-r Cartesian tensor

- a rank-r array of real numbers $T_{i_1 i_2 \dots i_r}$ as before
- transforms according to $T'_{i_1 i_2 \dots i_r} = L_{i_1 j_1} L_{i_2 j_2} \cdots L_{i_r j_r} T_{j_1 j_2 \dots j_r}$
- when vectors transform according to $V'_i = \mathbf{L}_{ij}V_j$

Principal axis system

- given a symmetric rank-2 tensor $\sigma_{ij} = \sigma_{ji}$ as the matrix $\boldsymbol{\sigma}$
- much simpler to work with tensor in the **principal axis system**
- column vectors of $\mathbf{L}$ are the eigenvectors $\vec{x}_i^{pas}$ as principal axes

Principal axis system

- given a symmetric rank-2 tensor $\sigma_{ij} = \sigma_{ji}$ as the matrix $\boldsymbol{\sigma}$
- much simpler to work with tensor in the **principal axis system**
- column vectors of $\mathbf{L}$ are the eigenvectors $\vec{x}_i^{pas}$ as principal axes

$$\boldsymbol{\sigma} = \mathbf{L} \begin{bmatrix} \sigma_1^{pas} & 0 & 0 \\ 0 & \sigma_2^{pas} & 0 \\ 0 & 0 & \sigma_3^{pas} \end{bmatrix} \mathbf{L}^T$$

- eigenvalues σ_i^{pas} are principal components, here conductivities
- parallel **cause** and **effect** in principal directions: eigenvalue eq.

Principal axis system

- given a symmetric rank-2 tensor $\sigma_{ij} = \sigma_{ji}$ as the matrix $\boldsymbol{\sigma}$
- much simpler to work with tensor in the **principal axis system**
- column vectors of $\mathbf{L}$ are the eigenvectors $\vec{x}_i^{pas}$ as principal axes

$$\boldsymbol{\sigma} = \mathbf{L} \begin{bmatrix} \sigma_1^{pas} & 0 & 0 \\ 0 & \sigma_2^{pas} & 0 \\ 0 & 0 & \sigma_3^{pas} \end{bmatrix} \mathbf{L}^T$$

- eigenvalues σ_i^{pas} are principal components, here conductivities
- parallel **cause** and **effect** in principal directions: eigenvalue eq.

$$\vec{J} = \boldsymbol{\sigma}\vec{E} \qquad \text{substitute } \vec{E} = \vec{x}_i^{pas}$$

$$\vec{J} = \boldsymbol{\sigma}\vec{x}_i^{pas} \qquad \text{eigenvalue eq. } \boldsymbol{\sigma}\vec{x}_i^{pas} = \sigma_i^{pas}\vec{x}_i^{pas}$$

$$\vec{J} = \sigma_i^{pas}\vec{x}_i^{pas} \qquad \text{substitute back } \vec{x}_i^{pas} = \vec{E}$$

$$\vec{J} = \sigma_i^{pas}\vec{E} \qquad \text{proportionality is a scalar } \sigma_i^{pas}$$

Summary of lecture 2

Rotations

- simplify description of anisotropic materials
- rotated axis vectors $\vec{x}'_i = \mathbf{L}\vec{x}_i$ are column vectors of $\mathbf{L}$
- active $\mathbf{L}\vec{v}$ equivalent to inverse passive rot of coord syst
- $\mathbf{L}$ transforms tensors into new coord syst as $\mathbf{LTL}^T$

Principal axis system

- can always find a rotation that diagonalises a (symmetric) tensor
- eigenvectors of matrix are the **principal axes**
- eigenvalues of the matrix are the **principal tensor components**
- cause and effect are parallel in the principal directions

NOTICE OF LECTURE RECORDING

- This session is being recorded and will be available for students to view on-demand. The recording will be stored in the Panopto cloud and will be accessible using your SSO via Canvas/WebLearn (delete as appropriate). Access to this recording is restricted to students in this year group and registered on this course.

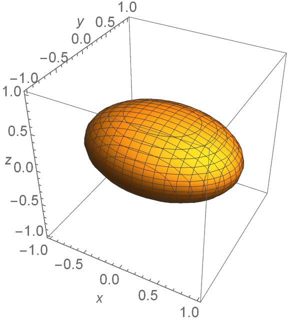
- Please be aware that all screen activity, including any active webcams/mics that are visible and/or audible, may be recorded.

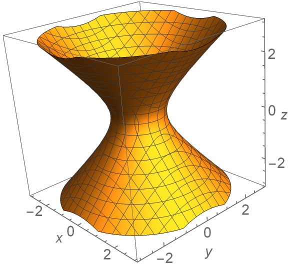
For more information about lecture recording at the University, please consult the University's Lecture Recording Policy.

If you have any questions or concerns, please email **replay@it.ox.ac.uk**

Visualisation and crystal symmetries

- rotations are crucial for treating anisotropy
- rotation matrices are very useful for computations
- **but** tensors rather abstract objects $\to$ visualisation
- we now introduce intuitive visualisations of tensors



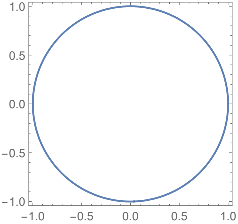


- single crystals have high symmetry
- this manifests in tensor properties

Reminder: surfaces via implicit equations

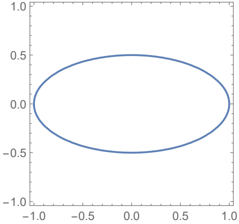
2D circle

$x^2 + y^2 = 1$



2D ellipse

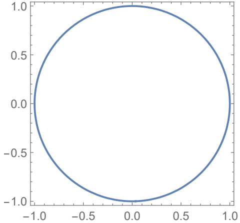
$x^2/a^2 + y^2/b^2 = 1$



Reminder: surfaces via implicit equations

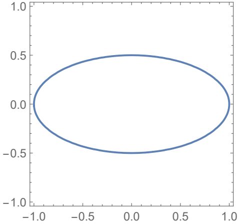
2D circle

$x^2 + y^2 = 1$



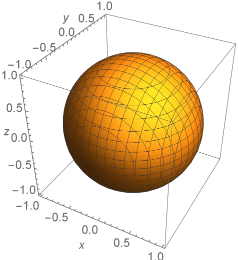
2D ellipse

$x^2/a^2 + y^2/b^2 = 1$



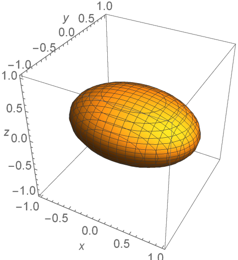
3D sphere

$x^2 + y^2 + z^2 = 1$



3D ellipsoid

$x^2/a^2 + y^2/b^2 + z^2/c^2 = 1$



Visualising tensors as surfaces

all $\vec{x} = (x, y, z)^T$ **that produce a parallel component** $\vec{x} \cdot \vec{v} = 1$

$$\boxed{\text{all } \vec{x}: \quad \vec{x}^T \mathbf{T} \vec{x} = \vec{x} \cdot \underbrace{(\mathbf{T}\vec{x})}_{\vec{v}} = 1 \qquad \text{for fixed } \mathbf{T}}$$

points $\vec{x}$ implicitly define a surface in 3D, representative of $\mathbf{T}$

Visualising tensors as surfaces

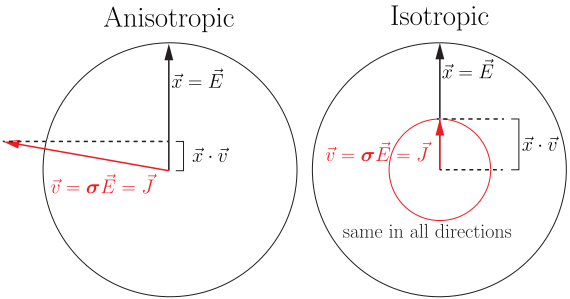
all $\vec{x} = (x, y, z)^T$ that produce a parallel component $\vec{x} \cdot \vec{v} = 1$

$$\text{all } \vec{x}: \quad \vec{x}^T \mathbf{T} \vec{x} = \vec{x} \cdot \underbrace{(\mathbf{T}\vec{x})}_{\vec{v}} = 1 \qquad \text{for fixed } \mathbf{T}$$

points $\vec{x}$ implicitly define a surface in 3D, representative of $\mathbf{T}$

Example: apply electric field $\vec{E} = \vec{x}$

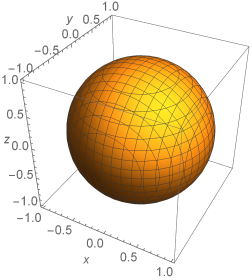
- then vector $\vec{v} = \boldsymbol{\sigma}\vec{E} = \vec{J}$ is current density
- scalar product $\vec{x} \cdot \vec{v} = \vec{E} \cdot \vec{J}$ is magnitude of parallel component



Examples of surfaces

isotropic material: T is scalar

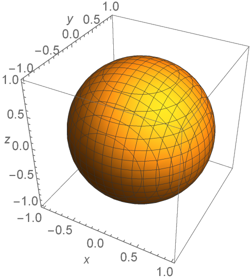
- simplifies $1 = \vec{x} \cdot (\mathbf{T}\vec{x}) = T\vec{x} \cdot \vec{x}$
- where $\vec{x} \cdot \vec{x} = x^2 + y^2 + z^2$
- surface: $1/T = x^2 + y^2 + z^2$
- sphere of radius $\sqrt{1/T}$



Examples of surfaces

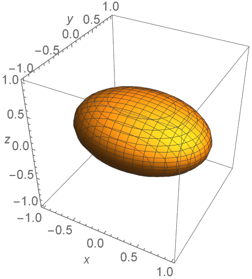
isotropic material: T is scalar

- simplifies $1 = \vec{x} \cdot (\mathbf{T}\vec{x}) = T\vec{x} \cdot \vec{x}$
- where $\vec{x} \cdot \vec{x} = x^2 + y^2 + z^2$
- surface: $1/T = x^2 + y^2 + z^2$
- sphere of radius $\sqrt{1/T}$



Principal Axis System and positive eigenvalues

- $\mathbf{T} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$
- then $\vec{v} = \mathbf{T}\vec{x} = (\lambda_1 x, \lambda_2 y, \lambda_3 z)^T$
- ellipsoid: $1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2$
- $a = \lambda_1^{-1/2}$, $b = \lambda_2^{-1/2}$, $c = \lambda_3^{-1/2}$



Representation quadrics

- T is symmetric $\rightarrow$ eigenvalues λ_1, λ_2, λ_3 are real
- ellipsoid if and only if $\lambda_1, \lambda_2, \lambda_3 > 0$ are positive
- generalisation of ellipsoid: quadric surfaces in PAS as

$$\boxed{1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2}$$

Representation quadrics

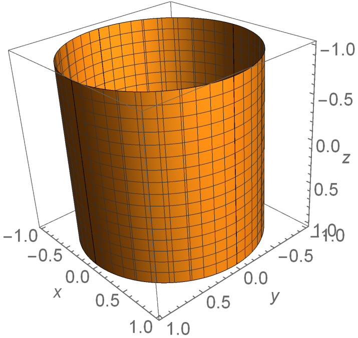
- T is symmetric $\rightarrow$ eigenvalues λ_1, λ_2, λ_3 are real
- ellipsoid if and only if $\lambda_1, \lambda_2, \lambda_3 > 0$ are positive
- generalisation of ellipsoid: quadric surfaces in PAS as

$$\boxed{1 = \lambda_1 x^2 + \lambda_2 y^2 + \lambda_3 z^2}$$

cylinder

one component zero

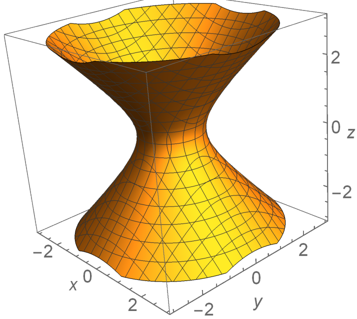
$(\lambda_1, \lambda_2, \lambda_3) = (1, 1, 0)$



hyperboloid

one component negative

$(\lambda_1, \lambda_2, \lambda_3) = (1, 1, -1)$



Rotational properties

start with: representation quadric of the tensor $\mathbf{T}$

$$1 = \vec{x}^T \mathbf{T} \vec{x} \qquad \text{substitute diagonal } \mathbf{T} = \mathbf{L}\mathbf{D}\mathbf{L}^T$$

$$1 = (\mathbf{L}^T \vec{x})^T \mathbf{D} (\mathbf{L}^T \vec{x}) \qquad \text{substitute new repr. coords. } \mathbf{L}^T \vec{x} = \vec{x}'$$

$$1 = (\vec{x}')^T \mathbf{D} \vec{x}' \qquad \text{this is: representation quadric of diagonal } \mathbf{D}$$

any symm. tensor $\mathbf{T}$: take $\mathbf{T}$ in PAS and rotate with eigenvectors

Rotational properties

start with: representation quadric of the tensor $\mathbf{T}$

$$1 = \vec{x}^T \mathbf{T} \vec{x} \qquad \text{substitute diagonal } \mathbf{T} = \mathbf{L}\mathbf{D}\mathbf{L}^T$$

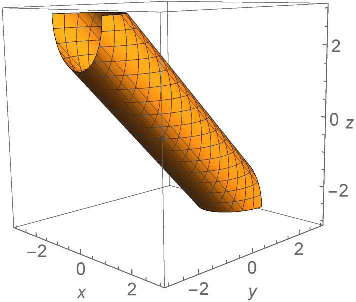
$$1 = (\mathbf{L}^T \vec{x})^T \mathbf{D} (\mathbf{L}^T \vec{x}) \qquad \text{substitute new repr. coords. } \mathbf{L}^T \vec{x} = \vec{x}'$$

$$1 = (\vec{x}')^T \mathbf{D} \vec{x}' \qquad \text{this is: representation quadric of diagonal } \mathbf{D}$$

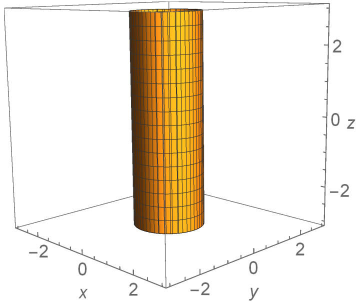
any symm. tensor $\mathbf{T}$: take $\mathbf{T}$ in PAS and rotate with eigenvectors

$$\mathbf{T} = \mathbf{L} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix} \mathbf{L}^T \qquad \mathbf{D} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

rotating $\mathbf{D}$ with 45° around $\vec{x}_1$

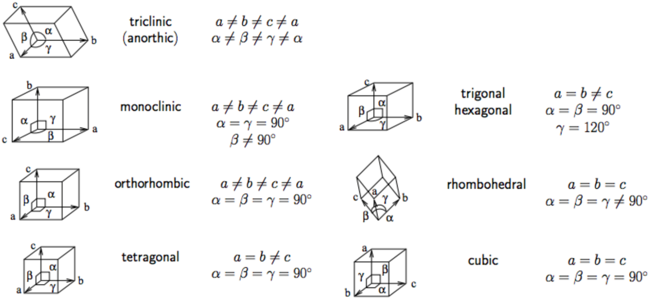


in Principal Axis System



Neumann's principle: *Any physical property of a crystal must include the symmetry elements of the point group of the crystal*

- symmetry may be higher, i.e., more invariants, but must include at least those symmetry elements
- symmetry of a rank-2 tensor depends only on crystal system, but not on particular point groups
- representation surface of a tensor also inherits these symmetry components
- crystal symmetry axes determine principal directions, i.e., the principal axis system



Effect of crystal structure

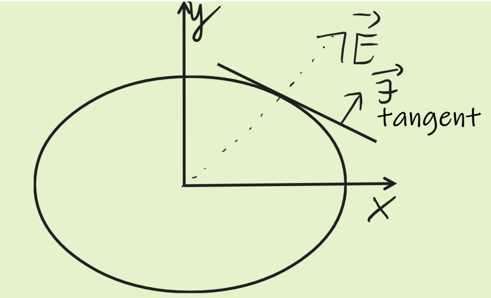
cryst. syst.	quadric orientation	params.	tensor
cubic	sphere	1	$\begin{bmatrix} T & 0 & 0 \\ 0 & T & 0 \\ 0 & 0 & T \end{bmatrix}$
tetragonal, hexagonal, trigonal	symm. around $\vec{x}_3$	2	$\begin{bmatrix} T_1 & 0 & 0 \\ 0 & T_1 & 0 \\ 0 & 0 & T_3 \end{bmatrix}$
orthorhombic	$\vec{x}_1$, $\vec{x}_2$, $\vec{x}_3$ parallel to diads	3	$\begin{bmatrix} T_1 & 0 & 0 \\ 0 & T_2 & 0 \\ 0 & 0 & T_3 \end{bmatrix}$
monoclinic	$\vec{x}_2$ parallel to diad	4	$\begin{bmatrix} T_{11} & 0 & T_{13} \\ 0 & T_{22} & 0 \\ T_{13} & 0 & T_{33} \end{bmatrix}$
triclinic	-	6	$\begin{bmatrix} T_{11} & T_{12} & T_{13} \\ T_{12} & T_{22} & T_{23} \\ T_{13} & T_{23} & T_{33} \end{bmatrix}$

- monoclinic: 3 eigenvalues + 1 angle
- triclinic: 3 eigenvalues + 3 angles
- others: crystal axes define tensor PAS

Radius normal property

- recall the representation quadric surface $1 = \vec{x}^T \boldsymbol{\sigma} \vec{x}$
- in PAS it is $1 = \sigma_1 x^2 + \sigma_2 y^2 + \sigma_3 z^2$ with conductivities $\sigma_1, \sigma_2, \sigma_3$
- the tangent plane vector is $\vec{t}(\vec{x}) = (2\sigma_1 x, 2\sigma_2 y, 2\sigma_3 z)^T$
- we compute as $\vec{t} = \vec{\nabla} F(x, y, z)$ where $0 = F(x, y, z) = \vec{x}^T \boldsymbol{\sigma} \vec{x} - 1$
- statement: $\vec{J} = \boldsymbol{\sigma} \vec{E}$ is parallel with $\vec{t}(\vec{E})$

$$\vec{J} = (\sigma_1 E_1, \sigma_2 E_2, \sigma_3 E_3)^T \qquad \vec{t}(\vec{E}) = 2(\sigma_1 E_1, \sigma_2 E_2, \sigma_3 E_3)^T$$



Summary of lecture 3

Visualisation of tensors

- applicable to symmetric rank-2 tensors
- surface: collection of points that satisfy quadric equation
- depending on eigenvalues of tensor we get different quadrics
- quadric surfaces: sphere, ellipsoid, hyperboloid, cylinder etc.
- quadrics transform naturally when transforming tensors

Effect of crystal structure

- Neumann's principle: physical properties of crystals must include cryst. symmetries
- therefore tensors include crystal symmetries via eigenvalues and eigenvectors
- these symmetries are also included by representation quadrics

NOTICE OF LECTURE RECORDING

- This session is being recorded and will be available for students to view on-demand. The recording will be stored in the Panopto cloud and will be accessible using your SSO via Canvas/WebLearn (delete as appropriate). Access to this recording is restricted to students in this year group and registered on this course.

- Please be aware that all screen activity, including any active webcams/mics that are visible and/or audible, may be recorded.

For more information about lecture recording at the University, please consult the University's Lecture Recording Policy.

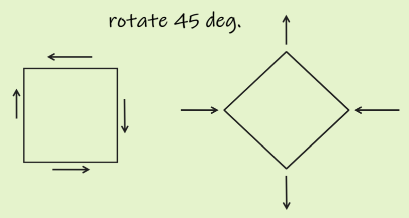
If you have any questions or concerns, please email **replay@it.ox.ac.uk**

Applications of tensors

- now equipped with mathematical tools
- illustrated concepts on linear response in anisotropic materials
- there tensors expressed properties of materials
- example $\vec{J} = \boldsymbol{\sigma}\vec{E}$

some more advanced applications of tensors

- mechanical stress and strain: tensor no longer property
- thermal expansion: cause is scalar
- stiffness via Hooke's law: tensor no longer rank 2

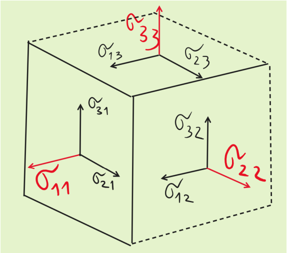


Stress tensor

- take any infinitesimally small cube of material
- traction vector $\vec{T}$ is force per unit area
- that acts on the plane represented by area vector $\vec{n}$

$$\vec{T} = \boldsymbol{\sigma}\vec{n} \qquad\qquad T_i = \sigma_{ij} n_j$$

- above guarantees rotational property $\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$ via Slide 19
- stress tensor is not a property of material: rather a variable
- equilibrium: tensile stresses equal but opposite $\boldsymbol{\sigma}(-\vec{n}) = -\vec{T}$

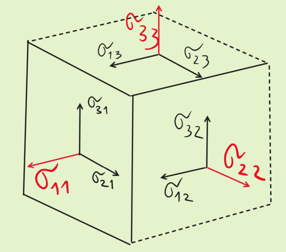


Stress tensor

- take any infinitesimally small cube of material
- traction vector $\vec{T}$ is force per unit area
- that acts on the plane represented by area vector $\vec{n}$

$$\vec{T} = \boldsymbol{\sigma}\vec{n} \qquad T_i = \sigma_{ij} n_j$$

- above guarantees rotational property $\boldsymbol{\sigma}' = \mathbf{L}\boldsymbol{\sigma}\mathbf{L}^T$ via Slide 19
- stress tensor is not a property of material: rather a variable
- equilibrium: tensile stresses equal but opposite $\boldsymbol{\sigma}(-\vec{n}) = -\vec{T}$



Warning: row vector convention

- often **row vectors** as $\vec{T}^T = \vec{n}^T \boldsymbol{\sigma}_{row}$
- need to use transpose $\boldsymbol{\sigma}_{row} = \boldsymbol{\sigma}^T$
- need to use inverse rotation $\mathbf{L}^T$ for row vectors
- possible confusion: $\mathbf{L}^T$ is inverse rotation in our convention

Equilibrium: conservation of angular momentum

- decompose any matrix into symm. and antisymm. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$
- we can define $2\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\sigma}^T$ and $2\boldsymbol{\sigma}^a = \boldsymbol{\sigma} - \boldsymbol{\sigma}^T$
- **Cauchy:** conservation of ang. mom. $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^s$ is symmetric

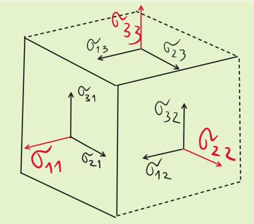
$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} =$$

Equilibrium: conservation of angular momentum

- decompose any matrix into symm. and antisymm. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$
- we can define $2\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\sigma}^T$ and $2\boldsymbol{\sigma}^a = \boldsymbol{\sigma} - \boldsymbol{\sigma}^T$
- **Cauchy:** conservation of ang. mom. $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^s$ is symmetric

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \underbrace{\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}}_{\text{tensile}}$$

positive: tensile
negative: compressive

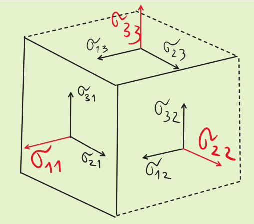


Equilibrium: conservation of angular momentum

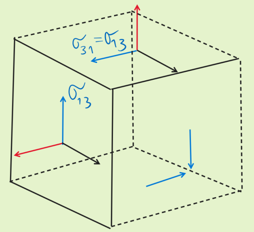
- decompose any matrix into symm. and antisymm. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$
- we can define $2\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\sigma}^T$ and $2\boldsymbol{\sigma}^a = \boldsymbol{\sigma} - \boldsymbol{\sigma}^T$
- **Cauchy:** conservation of ang. mom. $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^s$ is symmetric

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \underbrace{\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}}_{\text{tensile}} + \underbrace{\begin{bmatrix} 0 & \sigma^s_{12} & \sigma^s_{13} \\ \sigma^s_{12} & 0 & \sigma^s_{23} \\ \sigma^s_{13} & \sigma^s_{23} & 0 \end{bmatrix}}_{\text{shear}}$$

positive: tensile
negative: compressive



shear stress
conserves ang. mom.

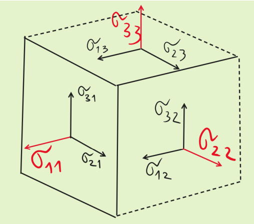


Equilibrium: conservation of angular momentum

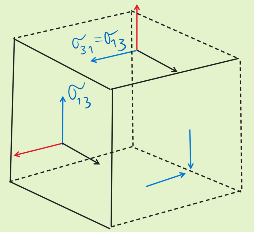
- decompose any matrix into symm. and antisymm. $\boldsymbol{\sigma} = \boldsymbol{\sigma}^s + \boldsymbol{\sigma}^a$
- we can define $2\boldsymbol{\sigma}^s = \boldsymbol{\sigma} + \boldsymbol{\sigma}^T$ and $2\boldsymbol{\sigma}^a = \boldsymbol{\sigma} - \boldsymbol{\sigma}^T$
- **Cauchy:** conservation of ang. mom. $\boldsymbol{\sigma} \equiv \boldsymbol{\sigma}^s$ is symmetric

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \underbrace{\begin{bmatrix} \sigma_{11} & 0 & 0 \\ 0 & \sigma_{22} & 0 \\ 0 & 0 & \sigma_{33} \end{bmatrix}}_{\text{tensile}} + \underbrace{\begin{bmatrix} 0 & \sigma^s_{12} & \sigma^s_{13} \\ \sigma^s_{12} & 0 & \sigma^s_{23} \\ \sigma^s_{13} & \sigma^s_{23} & 0 \end{bmatrix}}_{\text{shear}} + \underbrace{\begin{bmatrix} 0 & \sigma^a_{12} & \sigma^a_{13} \\ -\sigma^a_{12} & 0 & \sigma^a_{23} \\ -\sigma^a_{13} & -\sigma^a_{23} & 0 \end{bmatrix}}_{\text{rotation}}$$

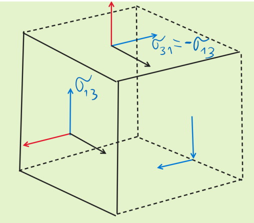
positive: tensile
negative: compressive



shear stress
conserves ang. mom.



rotation of the cube
zero in equilibrium



Principal stresses

- in equilibrium we can diagonalise $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
- but $\boldsymbol{\sigma}$ is not property of material: eigenvectors not necessarily related to crystal axes

stress type	principal comps.	example	tensor
triaxial	3 non-zero σ_k	-	$\mathrm{diag}(\sigma_1, \sigma_2, \sigma_3)$
biaxial	2 non-zero σ_k	force on thin plate	$\mathrm{diag}(\sigma_1, \sigma_2, 0)$
uniaxial	1 non-zero σ_k	pulling wire	$\mathrm{diag}(\sigma_1, 0, 0)$
hydrostatic	3 identical $\sigma_k < 0$	pressure p in fluid	$\mathrm{diag}(-p, -p, -p)$
pure shear	special biaxial	rod torsion	$\mathrm{diag}(-\sigma, \sigma, 0)$

Principal stresses

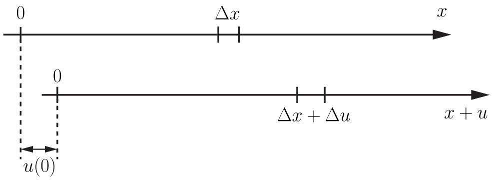
- in equilibrium we can diagonalise $\boldsymbol{\sigma} = \boldsymbol{\sigma}^T$
- but $\boldsymbol{\sigma}$ is not property of material: eigenvectors not necessarily related to crystal axes

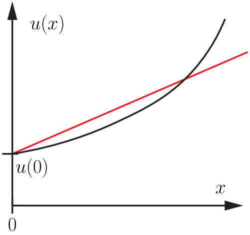
stress type	principal comps.	example	tensor
triaxial	3 non-zero σ_k	-	$\mathrm{diag}(\sigma_1, \sigma_2, \sigma_3)$
biaxial	2 non-zero σ_k	force on thin plate	$\mathrm{diag}(\sigma_1, \sigma_2, 0)$
uniaxial	1 non-zero σ_k	pulling wire	$\mathrm{diag}(\sigma_1, 0, 0)$
hydrostatic	3 identical $\sigma_k < 0$	pressure p in fluid	$\mathrm{diag}(-p, -p, -p)$
pure shear	special biaxial	rod torsion	$\mathrm{diag}(-\sigma, \sigma, 0)$

remark: how 'big' is the stress? no obvious metric as with vectors matrix invariants: $\mathrm{Tr}(A)$, determinant and matrix norms as $\mathrm{Tr}(A^T A)$

Strain in 1D

length of small element Δx increases due to stretching as $\Delta x + \Delta u$





$$\text{strain} = \frac{\text{increase in length}}{\text{original length}} = \lim_{\Delta x \to 0} \frac{\Delta u}{\Delta x} = \frac{\mathrm{d}u}{\mathrm{d}x}$$

- small element $(x, x + \Delta x)$ is increased to $(x + u, x + \Delta x + u + \Delta u)$
- strain ϵ is the derivative of displacement $u(x)$ wrt. position x
- homogeneous: derivative constant, global property
- Taylor expansion in homogeneous case: $u(x) - u(0) = \epsilon x$

Strain in 3D

- need to use vectors $\vec{u} = (u_1, u_2, u_3)^T$ and $\vec{x} = (x_1, x_2, x_3)^T$
- tensor: partial derivatives of displacement field wrt position

$$\tilde{\epsilon}_{ij} = \frac{\partial u_i}{\partial x_j}$$

- as before, antisymmetric part $(\tilde{\epsilon}_{ij} - \tilde{\epsilon}_{ji})/2$ is rotation

Strain in 3D

- need to use vectors $\vec{u} = (u_1, u_2, u_3)^T$ and $\vec{x} = (x_1, x_2, x_3)^T$
- tensor: partial derivatives of displacement field wrt position

$$\tilde{\epsilon}_{ij} = \frac{\partial u_i}{\partial x_j}$$

- as before, antisymmetric part $(\tilde{\epsilon}_{ij} - \tilde{\epsilon}_{ji})/2$ is rotation
- strain is a symmetric, rank-2 tensor

$$\epsilon_{ij} = (\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i})/2$$

$$\boldsymbol{\epsilon} = \underbrace{\begin{bmatrix} \epsilon_{11} & 0 & 0 \\ 0 & \epsilon_{22} & 0 \\ 0 & 0 & \epsilon_{33} \end{bmatrix}}_{\text{uniaxial extension}} + \underbrace{\begin{bmatrix} 0 & \epsilon_{12} & \epsilon_{13} \\ \epsilon_{12} & 0 & \epsilon_{23} \\ \epsilon_{13} & \epsilon_{23} & 0 \end{bmatrix}}_{\text{shear}}$$

- diagonals ϵ_{11}, ϵ_{22}, ϵ_{33} are uniaxial extensions per unit length
- off-diagonals are shear strains – coordinate syst. dependent
- homogeneous case: $\vec{u}(\vec{x}) - \vec{u}(0) = \boldsymbol{\epsilon}\vec{x}$

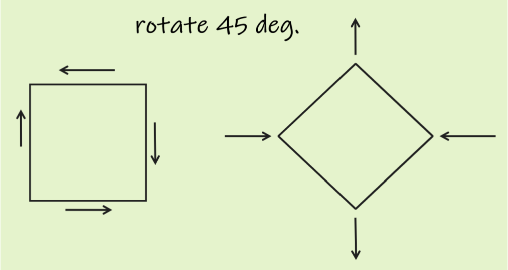
Pure shear stress and strain

assume the pure shear stress and strain tensors

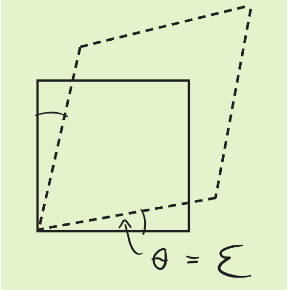
$$\boldsymbol{\sigma} = \begin{bmatrix} 0 & \sigma & 0 \\ \sigma & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \boldsymbol{\epsilon} = \begin{bmatrix} 0 & \epsilon & 0 \\ \epsilon & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- both can be diagonalised by a 45° rotation of the coord. syst.
- two eigenvalues $\pm\sigma$ and $\pm\epsilon$
- for strain $\epsilon = \epsilon_{12} = (\frac{\partial u_1}{\partial x_2} + \frac{\partial u_2}{\partial x_1})/2 = \tan(\theta) \approx \theta$

shear stress



shear strain



Strain tensor via thermal expansion

- material is heated up uniformly by ΔT
- strain tensor is proportional to this temperature
- proportionality: symmetric thermal expansion coefficients α_{ij}

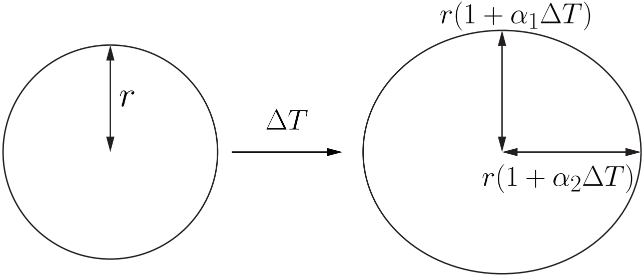
$$\boldsymbol{\epsilon} = \boldsymbol{\alpha} \Delta T \qquad \epsilon_{ij} = \alpha_{ij} \Delta T$$

Strain tensor via thermal expansion

- material is heated up uniformly by ΔT
- strain tensor is proportional to this temperature
- proportionality: symmetric thermal expansion coefficients α_{ij}

$$\boldsymbol{\epsilon} = \boldsymbol{\alpha}\Delta T \qquad \epsilon_{ij} = \alpha_{ij}\Delta T$$

- eigenvalues and eigenvectors contain crystal symmetries
- principal components $\epsilon_i = \alpha_i \Delta T$, e.g., along crystal axes
- α_i are typically positive, but can be negative
- volume expansion is $\Delta V \approx (\alpha_1 + \alpha_2 + \alpha_3)V\Delta T$ an invariant



Hooke's law and linear elasticity

in case of a 1D spring we have Hooke's law

$$F = kx$$

- can relate stress and strain in an elastic material
- linear mapping via rank-4 stiffness tensor c_{ijkl}

$$\sigma_{ij} = c_{ijkl}\,\epsilon_{kl}$$

Hooke's law and linear elasticity

in case of a 1D spring we have Hooke's law

$$F = kx$$

- can relate stress and strain in an elastic material
- linear mapping via rank-4 stiffness tensor c_{ijkl}

$$\sigma_{ij} = c_{ijkl}\, \epsilon_{kl}$$

- c_{ijkl} may generally have $3^4 = 81$ entries, but reduces to 21
- example: $\sigma_{ij} = \sigma_{ji}$, therefore $c_{ijkl} = c_{jikl}$
- example: $\epsilon_{kl} = \epsilon_{lk}$, therefore $c_{ijkl} = c_{ijlk}$
- in crystals this further reduces due to sytmmetries in ϵ_{kl}
- orthorhombic crystals: 9 entries, hexagonal crystals: 5, cubic: 3